

=> d ibib ab hitstr 1-3

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2001:935566 CAPLUS
 DOCUMENT NUMBER: 136:53633
 TITLE: Preparation of 7-phenyl-substituted tetracycline compounds and methods of treating tetracycline responsive states
 INVENTOR(S): Nelson, Mark; Rennie, Glen
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 29 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098259	A1	20011227	WO 2000-US16632	20000616
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LA, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 1999-154701P P 19990914

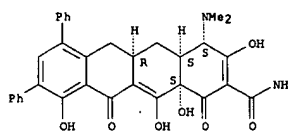
OTHER SOURCE(S): MARPAT 136:53633
 AB 7-Phenyl-substituted tetracycline compds., such as I [R4, R4' = alkyl; R5 = H, OH or prodrug moiety; R6, R6' = independently H, OH, alkyl, or taken together, alkenyl; R7 = (substituted)phenyl], and pharmaceutically acceptable salts thereof, are prepd. Thus, 7-phenylsancycline I (R4, R4' = Me; R5, R6, R6' = H; R7 = Ph) was produced from sancycline I (R4, R4' = Me; R5, R6, R6', R7 = H) through iodination at the 7-position with N-iodosuccinimide followed by palladium catalyzed coupling with phenylboronic acid in a combined 42% yield. An in vitro min. inhibitory concn. (MIC) assay used to det. the efficacy of I against common bacteria is described (no data). Addnl., methods of treating tetracycline responsive states, and pharmaceutical compns. contg. the 7-phenyl-substituted tetracycline compds are also described.

IT 330627-26-4P, 7,9-Diphenylsancycline
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of 7-phenyl-substituted tetracycline compds. and methods of treating tetracycline responsive states)

RN 330627-26-4 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7,9-diphenyl-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2002 ACS (Continued)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2001:935545 CAPLUS
 DOCUMENT NUMBER: 136:37446
 TITLE: 7-phenyl-substituted tetracycline compds. and methods of treating tetracycline responsive states
 INVENTOR(S): Nelson, Mark; Ismail, Mohamed Y.
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 32 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098236	A2	20011227	WO 2001-US19286	20010615
WO 2001098236	A3	20020328		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2000-212030P P 20000616
 US 2000-212471P P 20000616

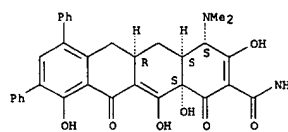
OTHER SOURCE(S): MARPAT 136:37446
 AB 7-Phenyl-substituted tetracycline compds. of formula I [R1, R2 = alkyl; R3 = H, OH or prodrug moiety; R4, R5 = independently H, OH, alkyl, or taken together, alkenyl; R6 = (substituted)phenyl] which are substantially free of positional isomers, are prepd. Thus, 7-(3-nitrophenyl)sancycline (II) was produced from sancycline through iodination at the 7-position with N-iodosuccinimide followed by palladium catalyzed coupling with 3-nitrophenylboronic acid in a combined 32% yield. An in vitro min. inhibitory concn. (MIC) assay used to det. the efficacy of tetracycline compds. against common bacteria (no data) is described. Addnl., methods of treating tetracycline responsive states, and pharmaceutical compns. contg. the 7-phenyl-substituted tetracycline compds are also described.

IT 330627-26-4P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (7-phenyl-substituted tetracycline compds. and methods of treating tetracycline responsive states)

RN 330627-26-4 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7,9-diphenyl-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS (Continued)



L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2001:208235 CAPLUS
 DOCUMENT NUMBER: 134:252206
 TITLE: Methods of preparing substituted tetracyclines with transition metal-based chemistries
 INVENTOR(S): Nelson, Mark L.; Rennie, Glen; Koza, Darrell J.
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 46 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019784	A1	20010322	WO 2000-US25040	20000913
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, ME, NO, NZ, PL, PT, RD, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

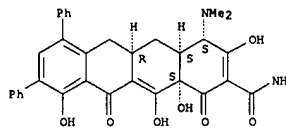
PRIORITY APPLN. INFO.: US 1999-154701P P 19990914
 US 2000-232091P P 20000912

OTHER SOURCE(S): CASREACT 134:252206; MARPAT 134:252206
 AB Substituted tetracycline derivatives were prepd. by combining a reactive tetracycline-based precursor and a reactive org. substituent precursor in the presence of a transition metal catalyst. In one embodiment of the invention, a substituted tetracycline compd. may be prepd. by combining a reactive tetracycline-based precursor compd. such as an arene tetracycline diazonium salt, and a reactive org. substituent precursor, e.g., alkenes, substituted alkenes, vinyl monomers, aroms. and heteroaroms., in the presence of a transition metal catalyst, such as palladium chloride, under conditions such that a tetracycline compd. substituted with the org. substituent is formed. Such compds. may optionally act as intermediates for making other compds., e.g., hydrogenation of unsatd. groups on the substituent. Thus, sancycline-HCl was treated with N-iodosuccinimide in concd. H2SO4 to give 61% 7-iodosancycline and 22% 7,9-diodosancycline. 7-iodosancycline was added to a degassed soln. of MeOH contg. Na2CO3 and Pd(OAc)2 and then 4-chlorophenylbromide added to give 7-(4-chlorophenyl)sancycline (I). Antibacterial activity of several derivs. was tabulated.

IT 330627-26-4P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (methods of prepg. substituted tetracyclines with transition metal-based chemistries)

RN 330627-26-4 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7,9-diphenyl-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2002 ACS (Continued)
 Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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 'HITSTR' IS NOT A VALID FORMAT FOR FILE 'MARPAT'

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 CAN ----- List of CA abstract numbers without answer numbers
 CBIB ----- AN, plus Compressed Bibliographic Data
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 SCAN ----- CC, SX, TI, ST, IT, and FQHIT (random display,
 no answer numbers)
 STD ----- BIB, IPC, and NCL (standard patent information)

IABS ----- ABS, indented with text labels
 IALL ----- ALL, indented with text labels
 IBIB ----- BIB, indented with text labels
 IMAX ----- MAX, indented with text labels
 ISTD ----- STD, indented with text labels
 OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations

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 at an arrow prompt (=>). Examples of formats include: "TI";
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L6 ANSWER 1 OF 1 MARPAT COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 134:252206 MARPAT
 TITLE: Methods of preparing substituted tetracyclines with transition metal-based chemistries
 INVENTOR(S): Nelson, Mark L.; Rennie, Glen; Koza, Darrell J.
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 46 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

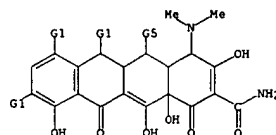
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019784	A1	20010322	WO 2000-US25040	20000913
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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PRIORITY APPLN. INFO.: US 1999-154701P 19990914
 US 2000-232091P 20000912

OTHER SOURCE(S): CASREACT 134:252206
 AB Substituted tetracycline derivatives were prep'd. by combining a reactive tetracycline-based precursor and a reactive org. substituent precursor in the presence of a transition metal catalyst. In one embodiment of the invention, a substituted tetracycline comp'd. may be prep'd. by combining a reactive tetracycline-based precursor comp'd. such as an arene tetracycline diazonium salt, and a reactive org. substituent precursor, e.g., alkenes, substituted alkenes, vinyl monomers, aroms. and heteroaroms., in the presence of a transition metal catalyst, such as palladium chloride, under conditions such that a tetracycline comp'd. substituted with the org. substituent is formed. Such comp'ds. may optionally act as intermediates for making other comp'ds., e.g., hydrogenation of unsat'd. groups on the substituent. Thus, tetracycline-HCl was treated with N-iodosuccinimide in conc'd. H₂SO₄ to give 61% 7-iodosancycline and 22% 7,9-diodosancycline. 7-iodosancycline was added to a degassed soln. of MeOH contg. Na₂CO₃ and Pd(OAc)₂ and then 4-chlorophenylbromide added to give 7-(4-chlorophenyl)sancycline (I). Antibacterial activity of several derivs. was tabulated.

MSTR 1

L6 ANSWER 1 OF 1 MARPAT COPYRIGHT 2002 ACS (Continued)



G1 = Ph
 MPL: disclosure

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L1 STRUCTURE UPLOADED

L2 0 S L1

L3 1 S L1 FULL

FILE 'CAPLUS' ENTERED AT 09:18:12 ON 01 AUG 2002

L4 3 S L3

FILE 'BEILSTEIN' ENTERED AT 09:18:52 ON 01 AUG 2002

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FILE 'MARPAT' ENTERED AT 09:19:05 ON 01 AUG 2002

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FILE 'USPATFULL' ENTERED AT 09:19:53 ON 01 AUG 2002

L7 0 S L3

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:51420 CAPLUS

DOCUMENT NUMBER: 136:102232

TITLE: Preparation of 7-substituted tetracycline derivatives for pharmaceutical use as antibacterial agents

INVENTOR(S): Nelson, Mark L.; Frechette, Roger; Viski, Peter; Ismail, Mohamed; Bowser, Todd; Bhatia, Beena; Messersmith, David; McIntyre, Laura; Koza, Darrell; Rennie, Glen; Sheahan, Paul; Hawkins, Paul; Verma, Atul; Warchol, Tad; Bandarage, Upul

PATENT ASSIGNEE(S): Trustees of Tufts College, USA; Paratek

SOURCE: Pharmaceutials, Inc.

PCT Int. Appl., 97 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004407	A2	20020117	WO 2001-US20766	20010629
WO 2002004407	A3	20020404		

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PRIORITY APPLN. INFO.: US 2000-216760P P 20000707
US 2001-275576P P 20010313

OTHER SOURCE(S): MARPAT 136:102232

AB 7-Substituted tetracycline derivs., such as I [R⁷ = NO₂, alkyl, alkenyl, alkynyl, aryl, alkoxy, alkylthio, alkylsulfanyl, alkylsulfonyl, alkylamino, arylalkyl, amino, arylalkenyl, arylalkynyl, aminoalkyl, etc.], were prep'd. for therapeutic use as antibacterial agents. Thus, 7-phenyltetracycline I (R⁷ = Ph) was prep'd. in 42% yield by arom. coupling reaction of 7-iodotetracycline I (R⁷ = I) with PhB(OH)₂ using Pd(OAc)₂ and Na₂CO₃ in MeOH under an argon atm. at r.t. for 2 h. The prep'd. tetracycline derivs. were tested for antibacterial activity against *Escherichia coli*, *Enterococcus hirae*, and *Staphylococcus aureus*.

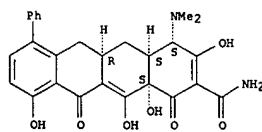
IT 263761-01-9P 389624-24-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

RN 263761-01-9 CAPLUS

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

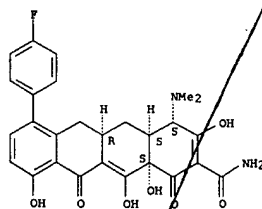
Absolute stereochemistry.



RN 263760-98-1 CAPLUS

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

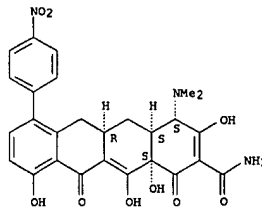


RN 263760-99-2 CAPLUS

CN 2-Naphthacenecarboxamide, 7-(4-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

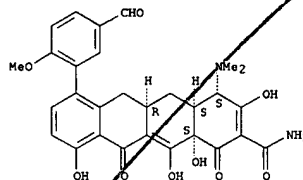
L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-24-2 CAPLUS

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(5-formyl-2-methoxyphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 263760-96-9P 263760-98-1P 263760-99-2P

263761-02-0P 374748-06-8P 380435-62-1P

380435-63-2P 380435-65-4P 380435-76-7P

389623-67-0P 389623-72-7P 389623-74-9P

389623-77-2P 389623-80-7P 389623-82-9P

389623-93-2P 389623-95-4P 389623-97-6P

389624-03-7P 389624-04-8P 389624-05-9P

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389624-45-7P 389624-54-8P 389624-55-9P

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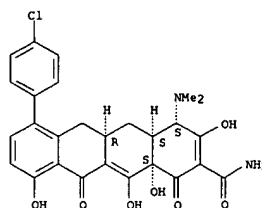
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389624-98-0P 389624-99-1P 389625-02-9P

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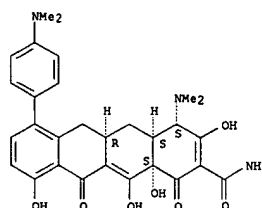
L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 263761-02-0 CAPLUS

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[4-(dimethylamino)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

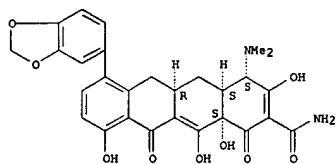


RN 374748-06-8 CAPLUS

CN 2-Naphthacenecarboxamide, 7-(1,3-benzodioxol-5-yl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

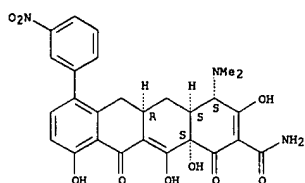
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-62-1 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(3-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

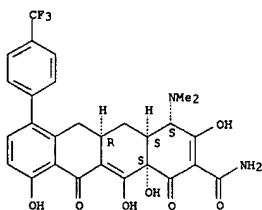
Absolute stereochemistry.



RN 380435-63-2 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(3-aminophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

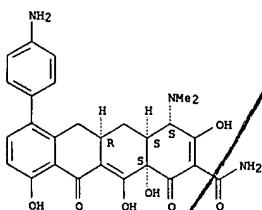
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389623-67-0 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-aminophenyl)-1,11-dioxo-, monohydrochloride, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

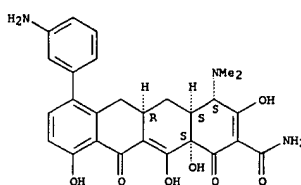


● HCl

RN 389623-72-1 CAPLUS
 CN Benzoic acid, 4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthaceny]-, methyl ester (9CI) (CA INDEX NAME)

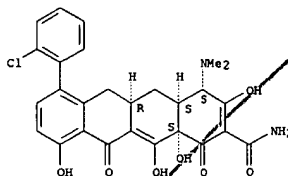
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-65-4 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(2-chlorophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

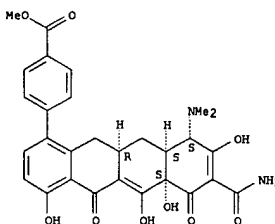
Absolute stereochemistry.



RN 380435-76-7 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[4-(trifluoromethyl)phenyl]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

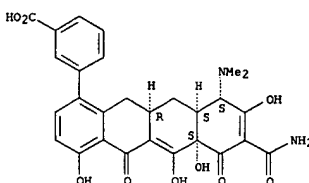
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389623-74-9 CAPLUS
 CN Benzoic acid, 3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthaceny]-, methyl ester (9CI) (CA INDEX NAME)

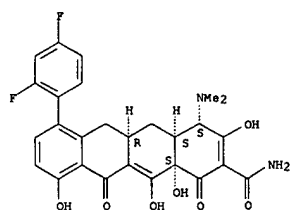
Absolute stereochemistry.



RN 389623-77-2 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(2,4-difluorophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

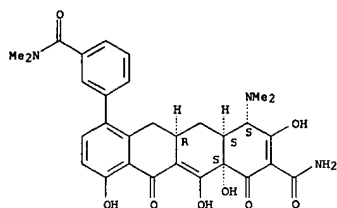
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389623-80-7 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-(3-[(dimethylamino)carbonyl]phenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

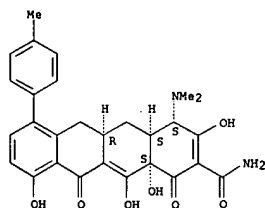
Absolute stereochemistry.



RN 389623-82-9 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-(2-ethoxyphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

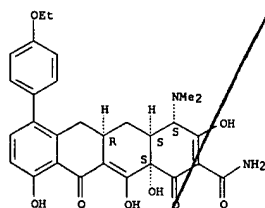
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389623-97-6 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-(4-ethoxyphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

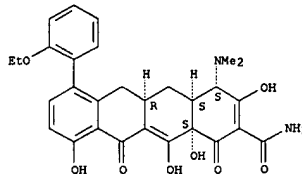
Absolute stereochemistry.



RN 389624-03-7 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(4-acetylphenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

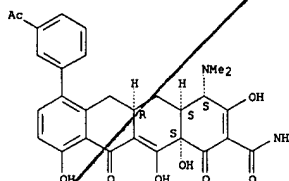
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389623-93-2 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(3-acetylphenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

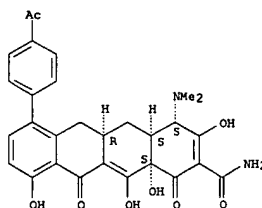
Absolute stereochemistry.



RN 389623-95-4 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-methylphenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

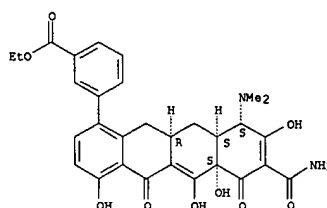
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-04-8 CAPLUS
 CN Benzoic acid, 3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, ethyl ester (9CI) (CA INDEX NAME)

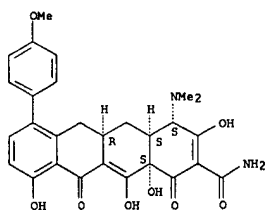
Absolute stereochemistry.



RN 389624-05-9 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-methoxyphenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

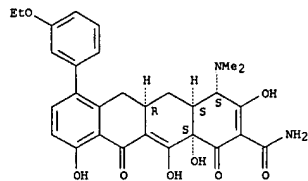
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-07-1 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-(3-methoxyphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

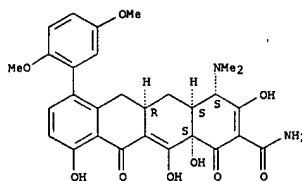
Absolute stereochemistry.



RN 389624-12-8 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(2,5-dimethoxyphenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

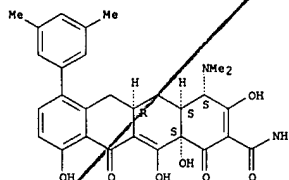
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-13-9 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-(3,5-dimethylphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

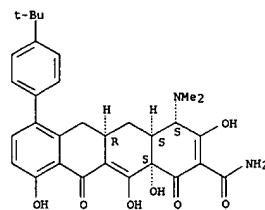
Absolute stereochemistry.



RN 389624-21-9 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-(4-(1,1-dimethylethyl)phenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

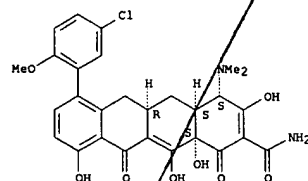
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-22-0 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(5-chloro-2-methoxyphenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

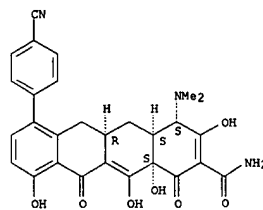
Absolute stereochemistry.



RN 389624-23-1 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(4-cyanophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

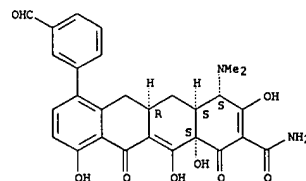
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-28-6 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-(3-formylphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

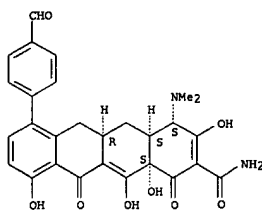
Absolute stereochemistry.



RN 389624-29-7 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-(4-formylphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

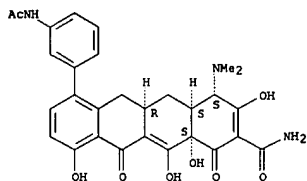
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-34-4 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-[(6aS,10S,10aS,11aR)-8-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-] (9CI) (CA INDEX NAME)

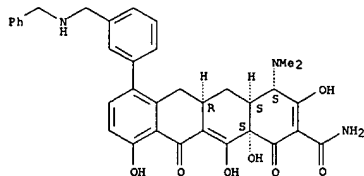
Absolute stereochemistry.



RN 389624-45-7 CAPLUS
 CN Benzoic acid, 4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]- (9CI) (CA INDEX NAME)

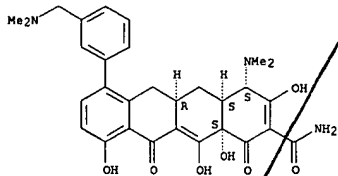
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



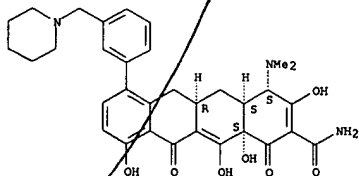
RN 389624-57-1 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



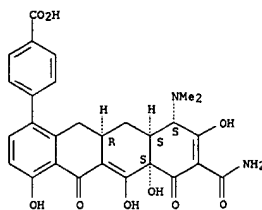
RN 389624-58-2 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



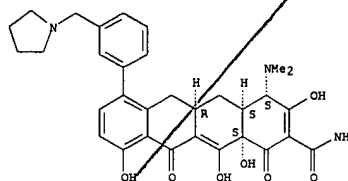
RN 389624-59-3 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-54-8 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]- (9CI) (CA INDEX NAME)

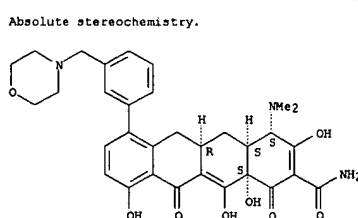
Absolute stereochemistry.



RN 389624-55-9 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]- (9CI) (CA INDEX NAME)

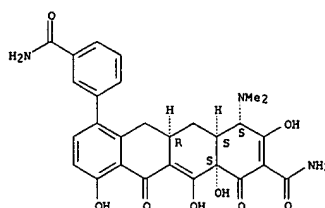
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-69-5 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]- (9CI) (CA INDEX NAME)

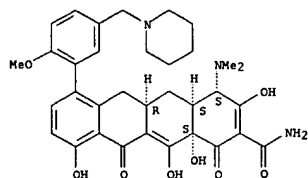
Absolute stereochemistry.



RN 389624-81-1 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]- (9CI) (CA INDEX NAME)

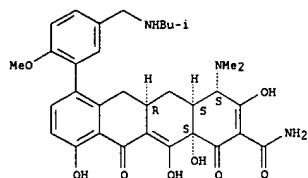
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-82-2 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[2-methoxy-5-[(2-methylpropyl)amino]methyl]phenyl-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

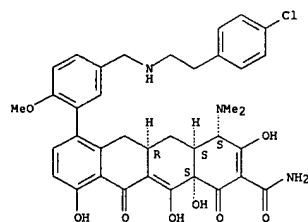
Absolute stereochemistry.



RN 389624-90-2 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-7-[5-[[[3-fluorophenyl]methyl]amino]methyl]-2-methoxyphenyl-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

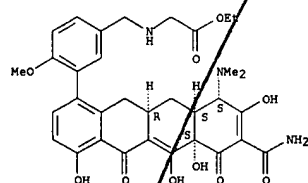
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-93-5 CAPLUS
 CN Glycine, N-[[[3-[[[6aS,10S,10aS,11aR]-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacene]-4-methoxyphenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

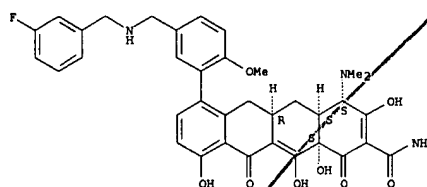
Absolute stereochemistry.



RN 389624-94-6 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-7-[5-[[[3-butoxypropyl]amino]methyl]-2-methoxyphenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

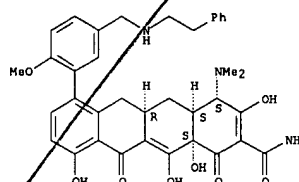
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-91-3 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[2-methoxy-5-[(2-phenylethyl)amino]methyl]phenyl-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

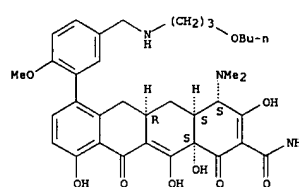
Absolute stereochemistry.



RN 389624-92-4 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 7-[5-[[[2-(4-chlorophenyl)ethyl]amino]methyl]-2-methoxyphenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

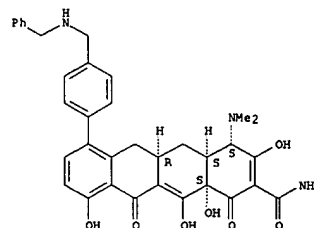
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-97-9 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[4-[[[phenylmethyl]amino]methyl]phenyl]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

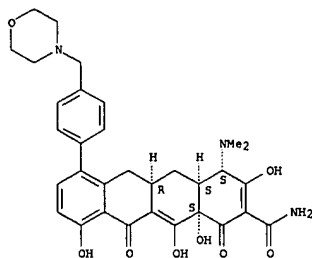
Absolute stereochemistry.



RN 389624-98-0 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[4-[[[4-morpholinylmethyl]phenyl]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

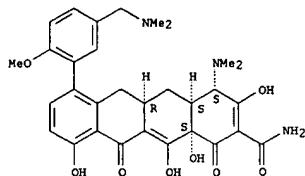
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-99-1 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-[5-[(dimethylamino)methyl]-2-methoxyphenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

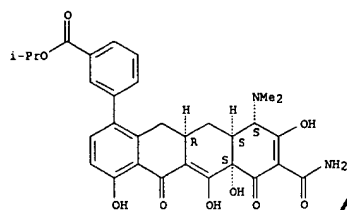
Absolute stereochemistry.



RN 389625-02-9 CAPLUS
 CN Phosphoramidic acid, [[3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]phenyl]methyl]pentyl-, diethyl ester (9CI) (CA INDEX NAME)

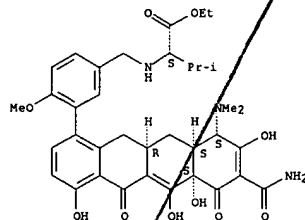
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389625-07-4 CAPLUS
 CN L-Valine, N-[[3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-4-methoxyphenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

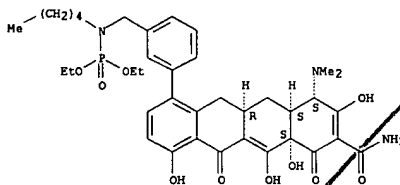
Absolute stereochemistry.



RN 389625-08-5 CAPLUS
 CN L-Valine, N-[[3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-4-methoxyphenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

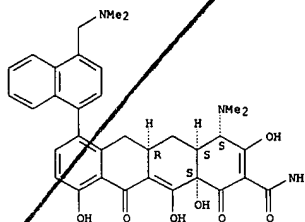
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389625-04-1 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-[4-[(dimethylamino)methyl]-1-naphthalenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

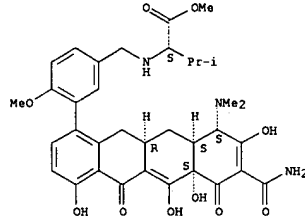
Absolute stereochemistry.



RN 389625-05-2 CAPLUS
 CN Benzoic acid, 3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

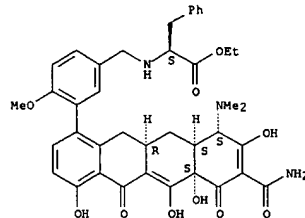
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389625-09-6 CAPLUS
 CN L-Phenylalanine, N-[[3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-4-methoxyphenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

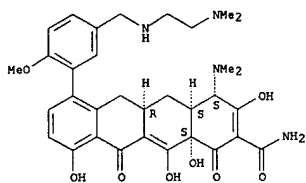
Absolute stereochemistry.



RN 389625-10-9 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-[5-[[[2-(dimethylamino)ethyl]amino]methyl]-2-methoxyphenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

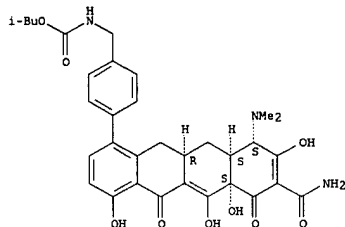
Absolute stereochemistry.

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



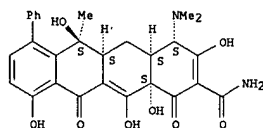
RN 389625-12-1 CAPLUS
 CN Carbamic acid, [[4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]phenyl]methyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



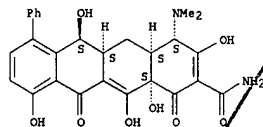
L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-7-phenyl-, (4S,4aS,5aS,6S,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



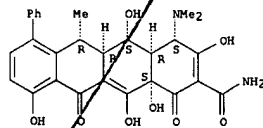
RN 389570-48-3 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-7-phenyl-, (4S,4aS,5aS,6S,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 389570-51-8 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-7-phenyl-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 389570-52-9 CAPLUS
 CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-7-(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

/Absolute stereochemistry.

L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2002:51417 CAPLUS
 DOCUMENT NUMBER: 136:102229
 TITLE: Preparation of 7,8 and 9-substituted tetracycline derivatives
 INVENTOR(S): Nelson, Mark L.; Koza, Darrell
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 26 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004404	A2	20020117	WO 2001-US20558	20010629
WO 2002004404	A3	20020613		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GM, GR, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002012170	A1	20020214	WO 2000-US21366	20000804

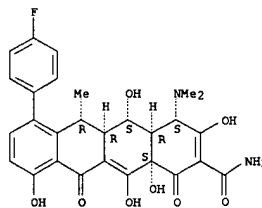
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PRIORITY APPL. INFO.: US 2000-216656P P 20000707
 WO 2000-US21366 W 20000804

OTHER SOURCE(S): MARPAT 136:102229
 AB The 7,8 and 9-substituted tetracycline derivs. 1 (R1 = H, OH; R2, R3 = H, Me, OH; R4 = H, alkenyl, alkynyl, Ph, halophenyl, acyl, phenylalkynyl, heteroaryl, dimethylamino; R5 = H, Ph, nitrophenyl, halo, alkynyl; R6 = H, amino, acetamide, alkynyl; at least one of R4, R5, and R6 is not H) and their pharmaceutically acceptable salts were as antibacterial agents. Thus, tetracycline underwent iodination with NIS to give a mixt. of 7- and 9-iodotetracycline, of which the 7- isomer was treated as Ph3 in presence of Pd(PPh3)2Cl2 and CuI to give 7-phenyltetracycline. I was screened to detpn. their in vitro antibacterial min. inhibitory concn. (no data).

IT 389570-44-9P 389570-48-3P 389570-51-8P 389570-52-9P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of 7,8 and 9-substituted tetracycline derivs. as antibacterial agents)
 RN 389570-44-9 CAPLUS

L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:935566 CAPLUS
 DOCUMENT NUMBER: 136:53633
 TITLE: Preparation of 7-phenyl-substituted tetracycline compounds and methods of treating tetracycline responsive states
 INVENTOR(S): Nelson, Mark; Rennie, Glen
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 29 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

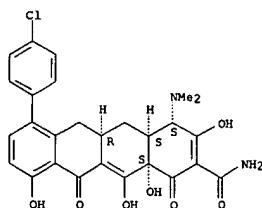
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098259	A1	20011227	WO 2000-US16632	20000616

V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, US, ES, FI, GB, GD, GE, GR, HU, IL, IN, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MW, MX, MY, NZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, T2, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPL. INFO.: US 1999-154701P P 19990914

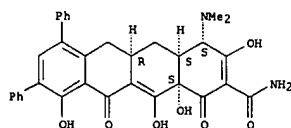
OTHER SOURCE(S): MARPAT 136:53633
 AB 7-Phenyl-substituted tetracycline compounds, such as I [R4, R4' = alkyl; R5 = H, OH or prodrug moiety; R6, R6' = independently H, OH, alkyl, or taken together, alkenyl; R7 = (substituted)phenyl], and pharmaceutically acceptable salts thereof, are prep'd. Thus, 7-phenylsancycline I (R4, R4' = Me; R5, R6, R6' = H; R7 = Ph) was produced from sancycline I (R4, R4' = Me; R5, R6, R6', R7 = H) through iodination at the 7-position with N-iodosuccinimide followed by palladium catalyzed coupling with phenylboronic acid in a combined 42% yield. An in vitro min. inhibitory concn. (MIC) assay used to det. the efficacy of I against common bacteria is described (no data). Addnl., methods of treating tetracycline responsive states, and pharmaceutical compns. contg. the 7-phenyl-substituted tetracycline compds are also described.
 IT 263760-96-9P, 7-Phenylsancycline 263760-98-1P, 7-(4-Fluorophenyl)sancycline 263760-99-2P, 7-(4-Chlorophenyl)sancycline 330627-26-4P, 7,9-Diphenylsancycline 380435-64-3P, 7-(2-Fluorophenyl)sancycline 380435-65-4P, 7-(2-Chlorophenyl)sancycline 380435-66-5P, 7-(2-Bromophenyl)sancycline 380435-67-6P, 7-(2-Iodophenyl)sancycline 380435-68-7P, 7-(3-Fluorophenyl)sancycline 380435-69-8P, 7-(3-Chlorophenyl)sancycline 380435-70-1P, 7-(3-Bromophenyl)sancycline 380435-72-3P, 7-(3-Iodophenyl)sancycline 380435-73-4P, 7-(4-Bromophenyl)sancycline 380435-74-5P, 7-(4-Iodophenyl)sancycline 380435-75-6P, 7-(4-Trichloromethylphenyl)sancycline 380435-76-7P, 7-(4-Trifluoromethylphenyl)sancycline 380435-77-8P, 7-(4-Tribromomethylphenyl)sancycline 380435-78-9P, 7-(4-Triiodomethylphenyl)sancycline
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



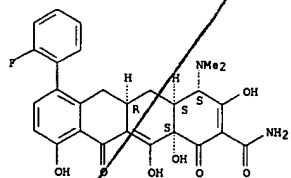
RN 330627-26-4 CAPLUS
 CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7,9-diphenyl-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-64-3 CAPLUS
 CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(2-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

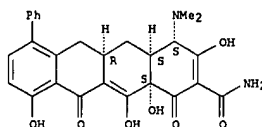


RN 380435-65-4 CAPLUS
 CN 2-Naphthacenecarboxamide, 7-(2-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-,

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of 7-phenyl-substituted tetracycline compds. and methods of treating tetracycline responsive states)

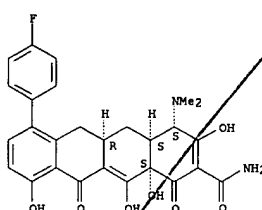
RN 263760-96-9 CAPLUS
 CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-phenyl-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 263760-98-1 CAPLUS
 CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

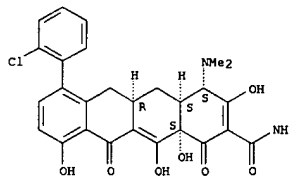


RN 263760-99-2 CAPLUS
 CN 2-Naphthacenecarboxamide, 7-(4-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

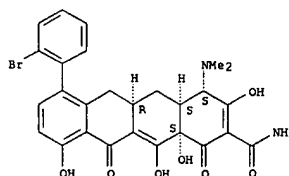
L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)
 (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



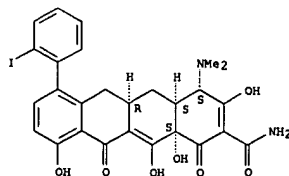
RN 380435-66-5 CAPLUS
 CN 2-Naphthacenecarboxamide, 7-(2-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-67-6 CAPLUS
 CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(2-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

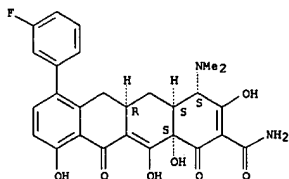
Absolute stereochemistry.



L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)

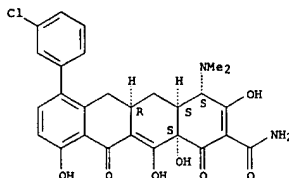
RN 380435-68-7 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-(3-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-69-8 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(3-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

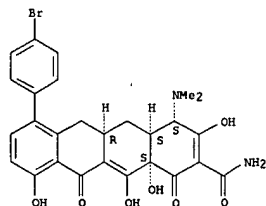
Absolute stereochemistry.



RN 380435-70-1 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(3-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

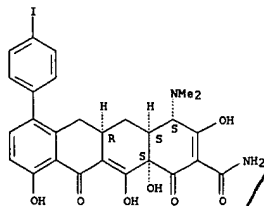
Absolute stereochemistry.

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-74-5 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

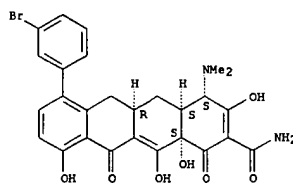
Absolute stereochemistry.



RN 380435-75-6 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(trichloromethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

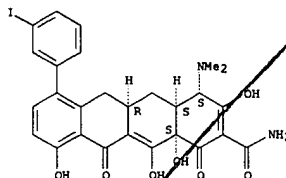
Absolute stereochemistry.

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-72-3 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(3-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

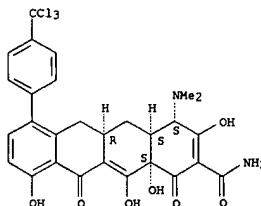
Absolute stereochemistry.



RN 380435-73-4 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(4-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

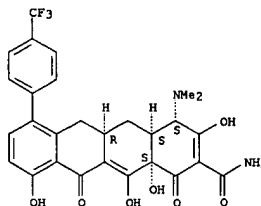
Absolute stereochemistry.

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-76-7 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(trifluoromethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

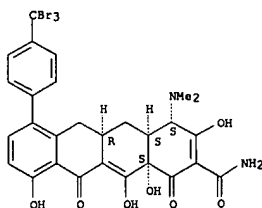
Absolute stereochemistry.



RN 380435-77-8 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(tribromomethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

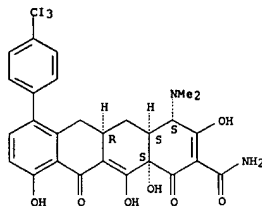
Absolute stereochemistry.

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-78-9 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[(4-(triiodomethyl)phenyl)-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

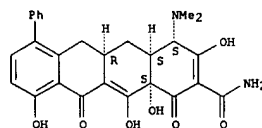


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)

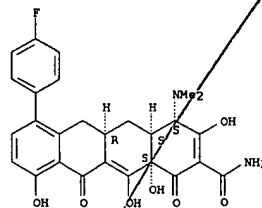
RN 263760-96-9 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-phenyl-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 263760-98-1 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-[(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 263760-99-2 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-[(4-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:93545 CAPLUS
 DOCUMENT NUMBER: 136:37446
 TITLE: 7-phenyl-substituted tetracycline compds. and methods of treating tetracycline responsive states
 INVENTOR(S): Nelson, Mark; Ismail, Mohamed Y.
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 32 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

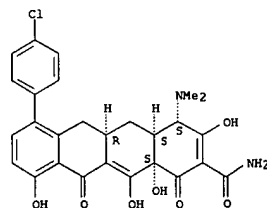
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098236	A2	20011227	WO 2001-0519286	20010615
WO 2001098236	A3	20020328		

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PRIORITY APPLN. INFO.: US 2000-212030P P 20000616
 US 2000-212471P P 20000616

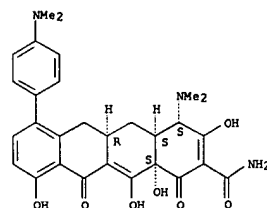
OTHER SOURCE(S): MARPAT 136:37446
 AB 7-Phenyl-substituted tetracycline compds. of formula I [R1, R2 = alkyl; R3 = H, OH or prodrug moiety; R4, R5 = independently H, OH, alkyl, or, taken together, alkenyl; R6 = (substituted)phenyl] which are substantially free of positional isomers, are prepd. Thus, 7-(3-nitrophenyl)sanclycine (II) was produced from sanclycine through iodination at the 7-position with N-iodosuccinimide followed by palladium catalyzed coupling with 3-nitrophenylboronic acid in a combined 32% yield. An in vitro min. inhibitory concn. (MIC) assay used to det. the efficacy of tetracycline compds. against common bacteria (no data) is described. Addnl., methods of treating tetracycline responsive states, and pharmaceutical compns. compg. the 7-phenyl-substituted tetracycline compds are also described.
 IT 263760-96-9P 263760-98-1P 263760-99-2P
 263761-02-0P 330627-26-4P 380435-62-1P
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 380435-66-5P 380435-67-6P 380435-68-7P
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 380435-88-1P 380435-89-2P 380435-91-6P
 380435-92-7P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (7-phenyl-substituted tetracycline compds. and methods of treating

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



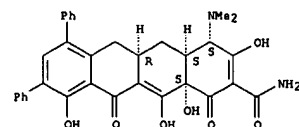
RN 263761-02-0 CAPLUS
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Absolute stereochemistry.



RN 330627-26-4 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7,9-diphenyl-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

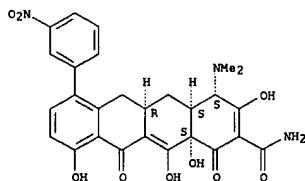
Absolute stereochemistry.



L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)

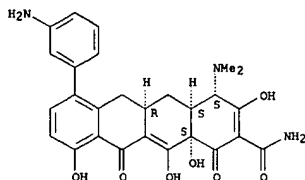
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 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(3-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-63-2 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(3-aminophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



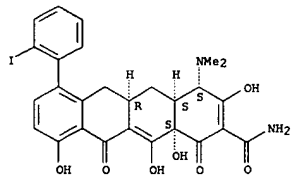
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 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-(2-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)

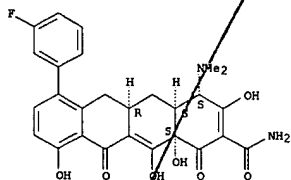
RN 380435-67-6 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(2-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-68-7 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-(3-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

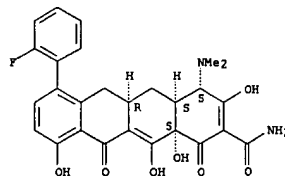
Absolute stereochemistry.



RN 380435-69-8 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(3-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

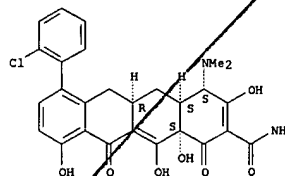
Absolute stereochemistry.

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



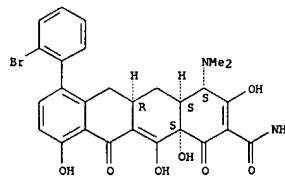
RN 380435-65-4 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(2-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

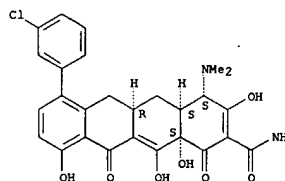


RN 380435-66-5 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(2-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

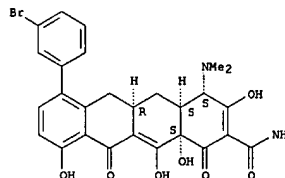


L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



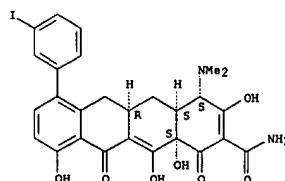
RN 380435-70-1 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 7-(3-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-72-3 CAPLUS
 CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(3-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

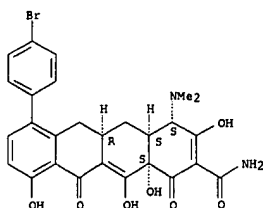


L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)

RN 380435-73-4 CAPLUS

CN 2-Naphthacene-3-carboxamide, 7-(4-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

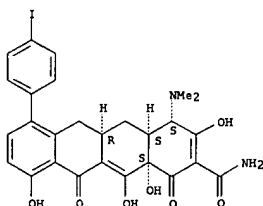
Absolute stereochemistry.



RN 380435-74-5 CAPLUS

CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

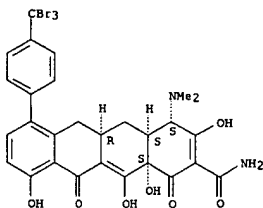


RN 380435-75-6 CAPLUS

CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-(trichloromethyl)phenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

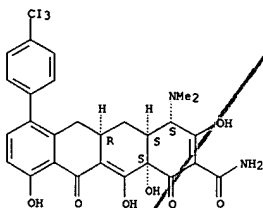
L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-78-9 CAPLUS

CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-(triiodomethyl)phenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

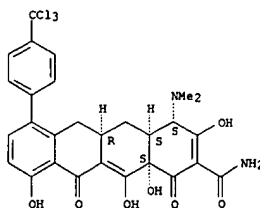


RN 380435-79-0 CAPLUS

CN 2-Naphthacene-3-carboxamide, 7-(2-aminophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

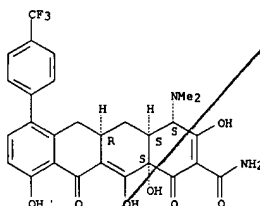
L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-76-7 CAPLUS

CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-(trifluoromethyl)phenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

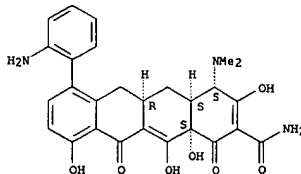


RN 380435-77-8 CAPLUS

CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-(tribromomethyl)phenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

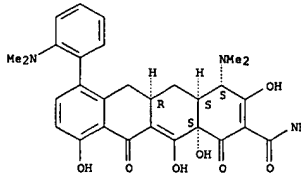
L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-80-3 CAPLUS

CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-[2-(dimethylamino)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

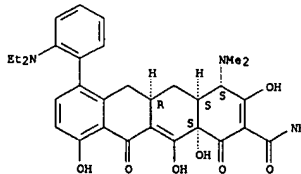
Absolute stereochemistry.



RN 380435-81-4 CAPLUS

CN 2-Naphthacene-3-carboxamide, 7-[2-(diethylamino)phenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

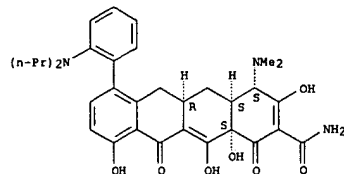


RN 380435-82-5 CAPLUS

CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-[2-(diethylamino)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

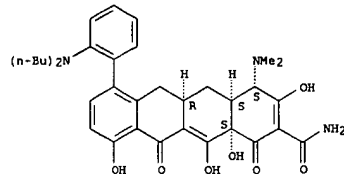
L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)
(4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-83-6 CAPLUS
CN 2-Naphthacene-3-carboxamide, 7-[(2S,3S,4S,5S)-2-(diethylamino)-3,4,5-trihydroxy-6-oxo-1,2,3,4-tetrahydronaphthalen-1-yl]-4-(dimethylamino)-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

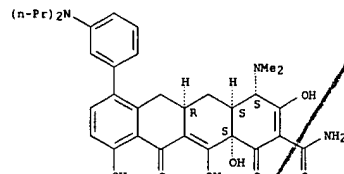
Absolute stereochemistry.



RN 380435-84-7 CAPLUS
CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-[(2S,3S,4S,5S)-2-(diethylamino)-3,4,5-trihydroxy-6-oxo-1,2,3,4-tetrahydronaphthalen-1-yl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

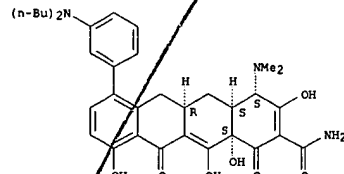
Absolute stereochemistry.

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-87-0 CAPLUS
CN 2-Naphthacene-3-carboxamide, 7-[(2S,3S,4S,5S)-2-(diethylamino)-3,4,5-trihydroxy-6-oxo-1,2,3,4-tetrahydronaphthalen-1-yl]-4-(dimethylamino)-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

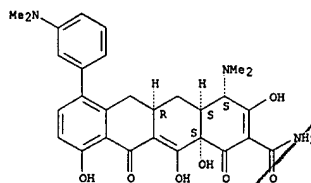
Absolute stereochemistry.



RN 380435-88-1 CAPLUS
CN 2-Naphthacene-3-carboxamide, 7-[(4S,5aR,12aS)-4-(aminophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

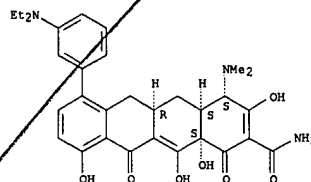
Absolute stereochemistry.

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-85-8 CAPLUS
CN 2-Naphthacene-3-carboxamide, 7-[(2S,3S,4S,5S)-2-(diethylamino)-3,4,5-trihydroxy-6-oxo-1,2,3,4-tetrahydronaphthalen-1-yl]-4-(dimethylamino)-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

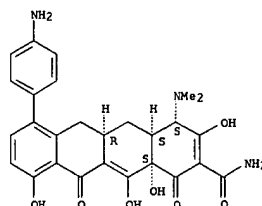
Absolute stereochemistry.



RN 380435-86-9 CAPLUS
CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-[(2S,3S,4S,5S)-2-(diethylamino)-3,4,5-trihydroxy-6-oxo-1,2,3,4-tetrahydronaphthalen-1-yl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

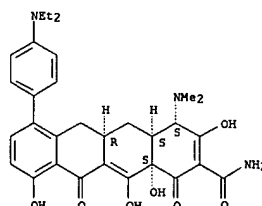
Absolute stereochemistry.

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-89-2 CAPLUS
CN 2-Naphthacene-3-carboxamide, 7-[(2S,3S,4S,5S)-2-(diethylamino)-3,4,5-trihydroxy-6-oxo-1,2,3,4-tetrahydronaphthalen-1-yl]-4-(dimethylamino)-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

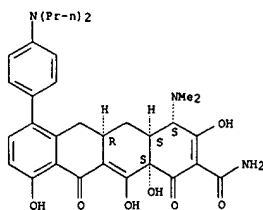
Absolute stereochemistry.



RN 380435-91-6 CAPLUS
CN 2-Naphthacene-3-carboxamide, 4-(dimethylamino)-7-[(2S,3S,4S,5S)-2-(diethylamino)-3,4,5-trihydroxy-6-oxo-1,2,3,4-tetrahydronaphthalen-1-yl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

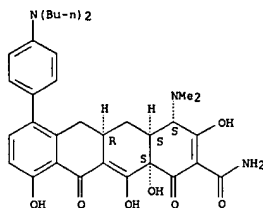
Absolute stereochemistry.

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-92-7 CAPLUS
CN 2-Naphthacene-1-carboxamide, 7-[(4-(dimethylamino)phenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-] (9CI) (CA INDEX NAME)

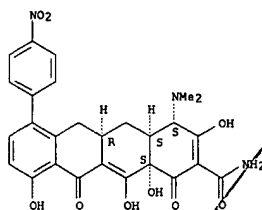
Absolute stereochemistry.



IT 263761-01-9 380435-93-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(7-phenyl-substituted tetracycline compds. and methods of treating tetracycline responsive states)
RN 263761-01-9 CAPLUS
CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

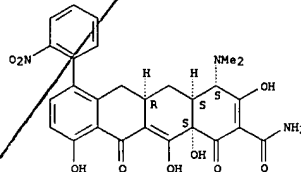
Absolute stereochemistry.

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-93-8 CAPLUS
CN 2-Naphthacene-1-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(2-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2002 ACS

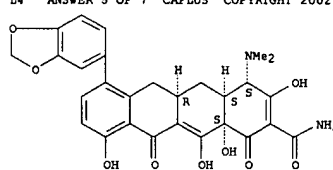
ACCESSION NUMBER: 2001:851102 CAPLUS
DOCUMENT NUMBER: 136:5854
TITLE: Preparation of 7-substituted fused ring tetracycline compounds as antibiotics
INVENTOR(S): Nelson, Mark L.; McIntyre, Laura
PATENT ASSIGNEE(S): Trustees of Tufts College, USA; Paratek Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: P13X02
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001087824	A2	20011122	WO 2001-0515068	20010510
WO 2001087824	A3	20020411		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
WO 2001098260	A1	20011227	WO 2000-0516672	20000616
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002045602	A1	20020418	US 2001-852908	20010510
PRIORITY APPLN. INFO.: US 2000-204158P P 20000515				

OTHER SOURCE(S): MARPAT 136:5854
AB The 7-substituted tetracycline derivs. I (R1 = H, OH, prodrug moiety; R2, R3 = alkyl; R4, R5 = H, OH, alkyl; R4R5 = alkenyl; Y, Y1 = C, N, O, S; X = CH2, CH2CH2) were prepd. as antibacterial agents. Thus, 7-(3,4-methylenedioxyphenyl)sancycline was prepd. from 7-iodosancycline (prepn. given) and 3,4-methylenedioxyphenylboronic acid. 7-(3,4-methylenedioxyphenyl)sancycline showed good inhibition of Escherichia coli at 0.098 .mu.g/mL.
IT 374748-06-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 7-substituted fused ring tetracycline compds. as antibiotics)
RN 374748-06-8 CAPLUS
CN 2-Naphthacene-1-carboxamide, 7-(1,3-benzodioxol-5-yl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



=> d ibib ab hitstr

LS ANSWER 1 OF 1 USPATFULL

ACCESSION NUMBER: 2002:85560 USPATFULL
TITLE: 7-substituted fused ring tetracycline compounds
INVENTOR(S): Nelson, Mark L., Wellesley, MA, UNITED STATES
McIntyre, Laura, Cambridge, MA, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002045602	A1	20020418
APPLICATION INFO.:	US 2001-852908	A1	20010510 (9)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2000-204158P	20000515 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	LAHIVE & COCKFIELD, 28 STATE STREET, BOSTON, MA, 02109	
NUMBER OF CLAIMS:	18	
EXEMPLARY CLAIM:	1	
LINE COUNT:	959	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

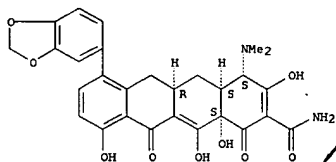
AB 7-substituted fused ring tetracycline compounds, methods of treating
tetracycline responsive states, and pharmaceutical compositions
containing the 7-substituted fused ring tetracycline compounds are
described.

IT 374748-06-8P
(prepn. of 7-substituted fused ring tetracycline compds. as
antibiotics)

RN 374748-06-8 USPATFULL

CN 2-Naphthacene-carboxamide, 7-(1,3-benzodioxol-5-yl)-4-(dimethylamino)-
1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-,
(4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d ibib ab fqhit 1-6

L6 ANSWER 1 OF 6 MARPAT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 136:102232 MARPAT
 TITLE: Preparation of 7-substituted tetracycline derivatives for pharmaceutical use as antibacterial agents
 INVENTOR(S): Nelson, Mark L.; Frachette, Roger; Viski, Peter; Ismail, Mohamed; Bowser, Todd; Bhatia, Beena; Messersmith, David; McIntyre, Laura; Koza, Darrell; Rennie, Glen; Sheahan, Paul; Hawkins, Paul; Verma, Atul; Warchol, Tad; Bandarage, Upul
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA; Paratek Pharmaceuticals, Inc.
 SOURCE: PCT Int. Appl., 97 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

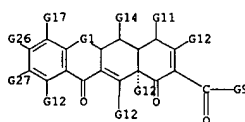
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004407	A2	20020117	WO 2001-US20766	20010629
WO 2002004407	A3	20020404		

V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:
 US 2000-216760P 20000707
 US 2001-275576P 20010313

AB 7-Substituted tetracycline derivs., such as I (R7 = NO2, alkyl, alkenyl, alkynyl, aryl, alkoxy, alkylthio, alkylsulfanyl, alkylsulfonyl, alkylamino, arylalkyl, amino, arylalkenyl, arylalkynyl, aminoalkyl, etc.), were prepd. for therapeutic use as antibacterial agents. Thus, 7-phenyltetracycline I (R7 = Ph) was prepd. in 42% yield by arom. coupling reaction of 7-iodotetracycline I (R7 = iodo) with PhB(OH)2 using Pd(OAc)2 and Na2CO3 in MeOH under an argon atm. at r.t. for 2 h. The prepd. tetracycline derivs. were tested for antibacterial activity against Escherichia coli, Enterococcus hirae, and Staphylococcus aureus.

MSTR 1



G1 = 21

L6 ANSWER 2 OF 6 MARPAT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 136:102229 MARPAT
 TITLE: Preparation of 7,8 and 9-substituted tetracycline derivatives
 INVENTOR(S): Nelson, Mark L.; Koza, Darrell
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 26 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004404	A2	20020117	WO 2001-US20558	20010629
WO 2002004404	A3	20020613		

V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:
 US 2000-216656P 20000707
 WO 2000-US21366 20000804

AB The 7,8 and 9-substituted tetracycline derivs. I (R1 = H, OH; R2, R3 = H, Me, OH; R4 = H, alkenyl, alkynyl, Ph, halophenyl, acyl, phenylalkynyl, heteroaryl, dimethylamino; R5 = H, Ph, nitrophenyl, halo, alkynyl; R6 = H, amino, acetamide, alkynyl; at least one of R4, R5, and R6 is not H) and their pharmaceutically acceptable salts were as antibacterial agents. Thus, tetracycline underwent iodination with IIS to give a mixt. of 7- and 9-iodotetracycline, of which the 7- isomer was treated as Ph3 in presence of Pd(PPh3)2Cl2 and CuI to give 7-phenyltetracycline. I were screened to detn. their in vitro antibacterial min. inhibitory concn. (no data).

MSTR 1

L6 ANSWER 1 OF 6 MARPAT COPYRIGHT 2002 ACS (Continued)

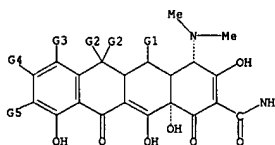


G9 = NH2
 G10 = Ak<EC (1-) C, BD (0-) D (0-) T> (SO (1-) G6)
 G11 = S1



G12 = OH
 G17 = Ph (SO (1-) G29)
 MPL: claim 1
 NTE: and pharmaceutically acceptable salts

L6 ANSWER 2 OF 6 MARPAT COPYRIGHT 2002 ACS (Continued)



G3 = Ph (SO (1-) G6)
 MPL: claim 1
 NTE: and pharmaceutically acceptable salts

L6 ANSWER 3 OF 6 MARPAT COPYRIGHT 2002 ACS

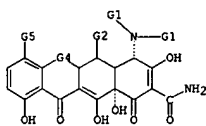
ACCESSION NUMBER: 136:53633 MARPAT
 TITLE: Preparation of 7-phenyl-substituted tetracycline compounds and methods of treating tetracycline responsive states
 INVENTOR(S): Nelson, Mark; Rennie, Glen
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 29 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098259	A1	20011227	WO 2000-US16632	20000616

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, BG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-154701P 19990914
 AB 7-Phenyl-substituted tetracycline compds., such as I [R4, R4' = alkyl; R5 = H, OH or prodrug moiety; R6, R6' = independently H, OH, alkyl, or taken together, alkenyl; R7 = (substituted)phenyl], and pharmaceutically acceptable salts thereof, are prepd. Thus, 7-phenylsancycline I (R4, R4' = Me; R5, R6, R6' = H; R7 = Ph) was produced from sancycline I (R4, R4' = Me; R5, R6, R6', R7 = H) through iodination at the 7-position with N-iodosuccinimide followed by palladium catalyzed coupling with phenylboronic acid in a combined 42% yield. An in vitro min. inhibitory concn. (MIC) assay used to det. the efficacy of I against common bacteria is described (no data). Addnl., methods of treating tetracycline responsive states, and pharmaceutical compns. contg. the 7-phenyl-substituted tetracycline compds are also described.

MSTR 1



G1 = Me
 G4 = 80

L6 ANSWER 4 OF 6 MARPAT COPYRIGHT 2002 ACS

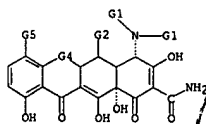
ACCESSION NUMBER: 136:37446 MARPAT
 TITLE: 7-phenyl-substituted tetracycline compds. and methods of treating tetracycline responsive states
 INVENTOR(S): Nelson, Mark; Ismail, Mohamed Y.
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 32 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098236	A2	20011227	WO 2001-US19286	20010615
WO 2001098236	A3	20020328		

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 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-212030P 20000616
 US 2000-212471P 20000616
 AB 7-Phenyl-substituted tetracycline compds. of formula I [R1, R2 = alkyl; R3 = H, OH or prodrug moiety; R4, R5 = independently H, OH, alkyl, or taken together, alkenyl; R6 = (substituted)phenyl] which are substantially free of positional isomers, are prepd. Thus, 7-(3-nitrophenyl)sancycline (II) was produced from sancycline through iodination at the 7-position with N-iodosuccinimide followed by palladium catalyzed coupling with 3-nitrophenylboronic acid in a combined 32% yield. An in vitro min. inhibitory concn. (MIC) assay used to det. the efficacy of tetracycline compds. against common bacteria (no data) is described. Addnl., methods of treating tetracycline responsive states, and pharmaceutical compns. contg. the 7-phenyl-substituted tetracycline compds are also described.

MSTR 1



G1 = Me
 G4 = 80



L6 ANSWER 3 OF 6 MARPAT COPYRIGHT 2002 ACS (Continued)



G5 = Ph (SO (1-) G6)
 MPL: claim 1
 NTE: and pharmaceutically acceptable salts

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 6 MARPAT COPYRIGHT 2002 ACS (Continued)

G5 = Ph (SO (1-) G6)
 MPL: claim 1
 NTE: and pharmaceutically acceptable salts

L6 ANSWER 5 OF 6 MARPAT COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 136:5854 MARPAT
 TITLE: Preparation of 7-substituted fused ring tetracycline compounds as antibiotics
 INVENTOR(S): Nelson, Mark L.; McIntyre, Laura
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA; Paratek Pharmaceuticals, Inc.
 SOURCE: PCT Int. Appl., 28 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001087824	A2	20011122	WO 2001-US15068	20010510
WO 2001087824	A3	20020411		

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 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 WO 2001098260 A1 20011227 WO 2000-US16672 20000616
 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 US 2002045602 A1 20020418 US 2001-852908 20010510
 PRIORITY APPLN. INFO.: US 2000-204158P 20000515

AB The 7-substituted tetracycline derivs. I (R1 = H, OH, prodrug moiety; R2, R3 = alkyl; R4, R5 = H, OH, alkyl, R4R5 = alkenyl; Y, Y1 = C, N, O, S; X = CH2, CH2CH2) were prepd. as antibacterial agents. Thus, 7-(3,4-methylenedioxyphenyl)sancycline was prepd. from 7-iodosancycline (prepn. given) and 3,4-methylenedioxyphenylboronic acid. 7-(3,4-Methylenedioxyphenyl)sancycline showed good inhibition of Escherichia coli at 0.098 .mu.g/mL.

MSTR 1

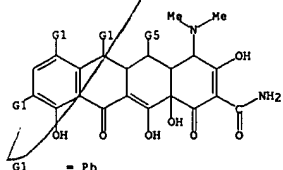
L6 ANSWER 6 OF 6 MARPAT COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 134:252206 MARPAT
 TITLE: Methods of preparing substituted tetracyclines with transition metal-based chemistries
 INVENTOR(S): Nelson, Mark L.; Rennie, Glen; Koza, Darrell J.
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 46 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019784	A1	20010322	WO 2000-US25040	20000913

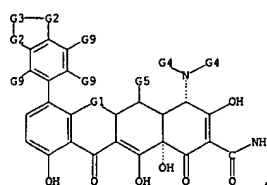
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 PRIORITY APPLN. INFO.: US 1999-154701P 19990914
 US 2000-232091P 20000912

OTHER SOURCE(S): CASREACT 134:252206
 AB Substituted tetracycline derivatives were prepd. by combining a reactive tetracycline-based precursor and a reactive org. substituent precursor in the presence of a transition metal catalyst. In one embodiment of the invention, a substituted tetracycline compd. may be prepd. by combining a reactive tetracycline-based precursor compd. such as an arene tetracycline diazonium salt and a reactive org. substituent precursor, e.g., alkenes, substituted alkenes, vinyl monomers, aroms. and heteroatoms, in the presence of a transition metal catalyst, such as palladium chloride, under conditions such that a tetracycline compd. substituted with the org. substituent is formed. Such compds. may optionally act as intermediates for making other compds., e.g., hydrogenation of unsatd. groups on the substituent. Thus, sancycline-HCl was treated with N-iodosuccinimide in concd. H2SO4 to give 61% 7-iodosancycline and 22% 7,9-diodosancycline. 7-iodosancycline was added to a degassed soln. of MeOH contg. Na2CO3 and Pd(OAc)2 and then 4-chlorophenylboronic acid added to give 7-(4-chlorophenyl)sancycline (I). Antibacterial activity of several derivs. was tabulated.

MSTR 1



L6 ANSWER 5 OF 6 MARPAT COPYRIGHT 2002 ACS (Continued)



G1 = 45

G8 = 45

G4 = Me

MPL: claim 1
 NTE: and pharmaceutically acceptable salts

L6 ANSWER 6 OF 6 MARPAT COPYRIGHT 2002 ACS (Continued)

MPL: disclosure

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

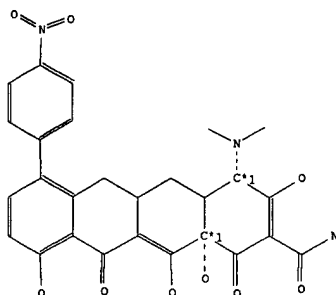
09/882,505

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L8 ANSWER 1 OF 5 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Beilstein Records (BRN): 8601328
 Chemical Name (CN): 7-(4-nitrophenyl)sancycline
 Autonom Name (AUN): 4-dimethylamino-3,10,12,12a-tetrahydroxy-7-(4-nitro-phenyl)-1,11-dioxo-1,4,4a,5,5a,6,11,12a-octahydro-naphthacene-2-carboxylic acid amide
 C27 H25 N3 O9
 Molec. Formula (MF): 535.51
 Molecular Weight (MW): 16311, 2817
 Lawson Number (LN): Stereo compound
 File Segment (FS): isocyclic
 Compound Type (CTYPE): 7289045
 Constitution ID (CONSID): 8099158
 Tautomer ID (TAUTID): 2000/10/24
 Entry Date (DED): 2000/10/24
 Update Date (DUPD): 2000/10/24



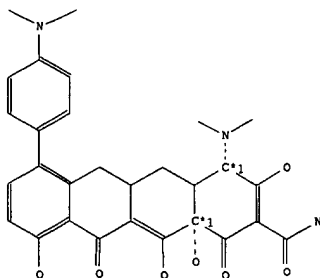
Atom/Bond Notes:
 1. CIP Descriptor: S

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1

L8 ANSWER 2 OF 5 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Beilstein Records (BRN): 8601284
 Chemical Name (CN): 7-(4-dimethylaminophenyl)sancycline
 Autonom Name (AUN): 4-dimethylamino-7-(4-dimethylamino-phenyl)-3,10,12,12a-tetrahydroxy-1,11-dioxo-1,4,4a,5,5a,6,11,12a-octahydro-naphthacene-2-carboxylic acid amide
 C29 H31 N3 O7
 Molec. Formula (MF): 533.58
 Molecular Weight (MW): 16311, 2817
 Lawson Number (LN): Stereo compound
 File Segment (FS): isocyclic
 Compound Type (CTYPE): 7288528
 Constitution ID (CONSID): 8096042
 Tautomer ID (TAUTID): 2000/10/24
 Entry Date (DED): 2000/10/24
 Update Date (DUPD): 2000/10/24



Atom/Bond Notes:
 1. CIP Descriptor: S

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

L8 ANSWER 1 OF 5 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL (Continued)

Code	Name	Occurrence
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Reaction:

RX
 Reaction ID: 8565125
 Reactant BRN: 8597075, 3978722
 Reactant: 7-iodosancycline, tributyl-(4-nitro-phenyl)-stannane
 Product BRN: 8601328
 Product: 7-(4-nitrophenyl)sancycline
 No. of Reaction Details: 1

Reaction Details:

RX
 Reaction RID: 8565125.1
 Reaction Classification: Preparation
 Yield: 83 percent (BRN=8601328)
 Reagent: CuI
 Catalyst: Pd(PPh3)2Cl2
 Reaction Type: Suzuki and Stille cross coupling
 Reference(s):
 1. Kozs, Darrell J., Org.Lett., CODEN: ORLEF7, 2(6), <2000>, 815 - 818; BABS-6238420

L8 ANSWER 2 OF 5 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL (Continued)

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Reaction:

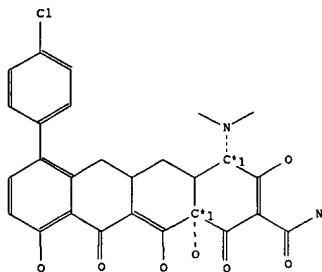
RX
 Reaction ID: 8560228
 Reactant BRN: 8597075, 3118297
 Reactant: 7-iodosancycline, (4-dimethylamino-phenyl)-boronic acid
 Product BRN: 8601284
 Product: 7-(4-dimethylaminophenyl)sancycline
 No. of Reaction Details: 1

Reaction Details:

RX
 Reaction RID: 8560228.1
 Reaction Classification: Preparation
 Yield: 28 percent (BRN=8601284)
 Reagent: CuI
 Catalyst: Pd(PPh3)2Cl2
 Reaction Type: Suzuki and Stille cross coupling
 Reference(s):
 1. Kozs, Darrell J., Org.Lett., CODEN: ORLEF7, 2(6), <2000>, 815 - 818; BABS-6238420

L8 ANSWER 3 OF 5 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Beilstein Records (BRN): 8600919
Chemical Name (CN): 7-(4-chlorophenyl)sancycline
Autonom Name (AUN): 7-(4-chloro-phenyl)-4-dimethylamino-3,10,12,12a-tetrahydroxy-1,11-dioxo-1,4,4a,5,5a,6,11,12a-octahydro-naphthacene-2-carboxylic acid amide
Molec. Formula (MF): C27 H25 Cl N2 O7
Molecular Weight (MW): 524.96
Lawson Number (LN): 16311, 2817
File Segment (FS): Stereo compound
Compound Type (CTYPE): isocyclic
Constitution ID (CONSID): 7288195
Tautomer ID (TAUTID): 8095683
Entry Date (DED): 2000/10/24
Update Date (DUPD): 2000/10/24



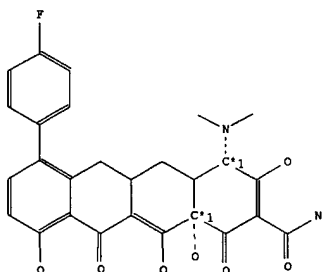
Atom/Bond Notes:
1. CIP Descriptor: S

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1

L8 ANSWER 4 OF 5 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Beilstein Records (BRN): 8600746
Chemical Name (CN): 7-(4-fluorophenyl)sancycline
Autonom Name (AUN): 4-dimethylamino-7-(4-fluoro-phenyl)-3,10,12,12a-tetrahydroxy-1,11-dioxo-1,4,4a,5,5a,6,11,12a-octahydro-naphthacene-2-carboxylic acid amide
Molec. Formula (MF): C27 H25 F N2 O7
Molecular Weight (MW): 508.50
Lawson Number (LN): 16311, 2817
File Segment (FS): Stereo compound
Compound Type (CTYPE): isocyclic
Constitution ID (CONSID): 7288071
Tautomer ID (TAUTID): 8095796
Entry Date (DED): 2000/10/24
Update Date (DUPD): 2000/10/24



Atom/Bond Notes:
1. CIP Descriptor: S

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

L8 ANSWER 3 OF 5 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL (Continued)

Code	Name	Occurrence
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Reaction:

RX
Reaction ID: 8559854
Reactant BRN: 8597075, 2936346
Reactant: 7-iodosancycline, (4-chloro-phenyl)-boronic acid
Product BRN: 8600919
Product: 7-(4-chlorophenyl)sancycline
No. of Reaction Details: 1

Reaction Details:

RX
Reaction RID: 8559854.1
Reaction Classification: Preparation
Yield: 42 percent (BRN=8600919)
Reagent: CuI
Catalyst: Pd(PPh3)2Cl2
Reaction Type: Suzuki and Stille cross coupling
Reference(s):
1. Kozs, Darrell J., Org.Lett., CODEN: ORLEF7, 2(6), <2000>, 815 - 818; BABS-6238420

L8 ANSWER 4 OF 5 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL (Continued)

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Reaction:

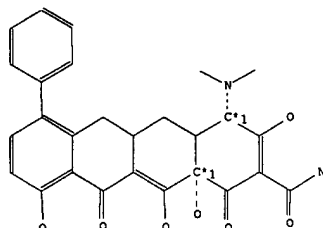
RX
Reaction ID: 8562281
Reactant BRN: 8597075, 3612877
Reactant: 7-iodosancycline, tributyl-(4-fluoro-phenyl)-stannane
Product BRN: 8600746
Product: 7-(4-fluorophenyl)sancycline
No. of Reaction Details: 1

Reaction Details:

RX
Reaction RID: 8562281.1
Reaction Classification: Preparation
Yield: 91 percent (BRN=8600746)
Reagent: CuI
Catalyst: Pd(PPh3)2Cl2
Reaction Type: Suzuki and Stille cross coupling
Reference(s):
1. Kozs, Darrell J., Org.Lett., CODEN: ORLEF7, 2(6), <2000>, 815 - 818; BABS-6238420

L8 ANSWER 5 OF 5 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Beilstein Records (BRN): 8598678
 Chemical Name (CN): 7-phenylsancycline
 Molec. Formula (MF): C27 H26 N2 O7
 Molecular Weight (MW): 490.51
 Lawson Number (LN): 16310, 2817
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): isocyclic
 Constitution ID (CONSID): 7286775
 Tautomer ID (TAUTID): 8094947
 Entry Date (DED): 2000/10/24
 Update Date (DUPD): 2000/10/24



Atom/Bond Notes:

1. CIP Descriptor: S

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

L8 ANSWER 5 OF 5 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL (Continued)

Code	Name	Occurrence
RX	Reaction Documents	2
RXPRO	Substance is Reaction Product	2

Reaction:

RX
 Reaction ID: 8606477
 Reactant BRN: 8597075, 970972
 Reactant: 7-iodosancycline, phenylboronic acid
 Product BRN: 8598678
 Product: 7-phenylsancycline
 No. of Reaction Details: 1

Reaction Details:

RX
 Reaction RID: 8606477.1
 Reaction Classification: Preparation
 Yield: 67 percent (BRN=8598678)
 Catalyst: Pd(OAc)₂
 Solvent: methanol
 Reaction Type: Suzuki and Stille cross coupling
 Reference(s):
 1. Koza, Darrell J., Org.Lett., CODEN: ORLEF7, 2(6), <2000>, 815 - 818;
 BABS-6238420

Reaction:

RX
 Reaction ID: 8562258
 Reactant BRN: 8597075, 3610571
 Reactant: 7-iodosancycline, tributyl-phenyl stannane
 Product BRN: 8598678
 Product: 7-phenylsancycline
 No. of Reaction Details: 1

Reaction Details:

RX
 Reaction RID: 8562258.1
 Reaction Classification: Preparation
 Yield: 87 percent (BRN=8598678)
 Reagent: CuI
 Catalyst: Pd(PPh₃)₂Cl₂
 Reaction Type: Suzuki and Stille cross coupling
 Reference(s):
 1. Koza, Darrell J., Org.Lett., CODEN: ORLEF7, 2(6), <2000>, 815 - 818;
 BABS-6238420

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L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2001:208235 CAPLUS
 DOCUMENT NUMBER: 134:252206
 TITLE: Methods of preparing substituted tetracyclines with transition metal-based chemistries
 INVENTOR(S): Nelson, Mark L.; Rennie, Glen; Koza, Darrell J.
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA
 SOURCE: PCT Int. Appl., 46 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019784	A1	20010322	WO 2000-US25040	20000913

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

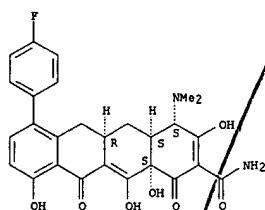
PRIORITY APPLN. INFO.:
 US 1999-154701P P 19990914
 US 2000-232091P P 20000912

OTHER SOURCE(S): CASREACT 134:252206; MARPAT 134:252206
 AB Substituted tetracycline derivatives were prepd. by combining a reactive tetracycline-based precursor and a reactive org. substituent precursor in the presence of a transition metal catalyst. In one embodiment of the invention, a substituted tetracycline compd. may be prepd. by combining a reactive tetracycline-based precursor compd. such as an arene tetracycline diazonium salt, and a reactive org. substituent precursor, e.g., alkenes, substituted alkenes, vinyl monomers, aroms. and heteroaroms., in the presence of a transition metal catalyst, such as palladium chloride, under conditions such that a tetracycline compd. substituted with the org. substituent is formed. Such compds. may optionally act as intermediates for making other compds., e.g., hydrogenation of unsatd. groups on the substituent. Thus, sancycline-HCl was treated with N-iodosuccinimide in concd. H2SO4 to give 61% 7-iodosancycline and 22% 7,9-diodosancycline. 7-iodosancycline was added to a degassed soln. of MeOH contg. Na2CO3 and Pd(OAc)2 and then 4-chlorophenylbromide added to give 7-(4-chlorophenyl)sancycline (I). Antibacterial activity of several derivs. was tabulated.

IT 263760-99-2P 330627-26-4P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (methods of prep. substituted tetracyclines with transition metal-based chemistries)

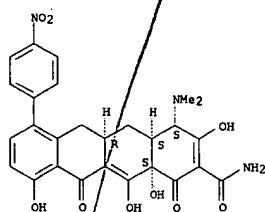
RN 263760-99-2 CAPLUS
 CN 2-Naphthacene-carboxamide, 7-(4-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



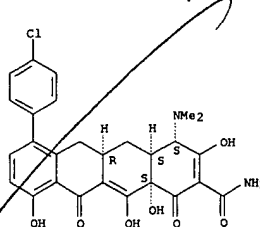
RN 263761-01-9 CAPLUS
 CN 2-Naphthacene-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



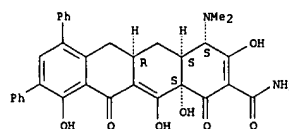
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)
 Absolute stereochemistry.



RN 330627-26-4 CAPLUS
 CN 2-Naphthacene-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7,9-diphenyl-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 263760-98-1P 263761-01-9P
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (methods of prep. substituted tetracyclines with transition metal-based chemistries)

RN 263760-98-1 CAPLUS
 CN 2-Naphthacene-carboxamide, 4-(dimethylamino)-7-(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:137899 CAPLUS
 DOCUMENT NUMBER: 132:279036
 TITLE: Synthesis of 7-Substituted Tetracycline Derivatives
 AUTHOR(S): Koza, Darrell J.
 CORPORATE SOURCE: Department of Science and Allied Health, Mount Ida College, Newton, MA, 02459, USA
 SOURCE: Organic Letters (2000), 2(6), 815-817
 CODEN: ORLE77; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

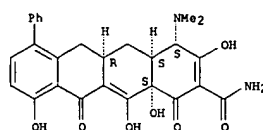
AB The synthesis of 7-substituted tetracycline derivs. has been accomplished in high yield from 7-halotetracyclines by modified Suzuki and Stille coupling protocols. These novel derivs. may serve as a new class of tetracycline antibiotics effective against multi-antibiotic-resistant bacteria.

IT 263760-96-9P 263760-98-1P 263760-99-2P
 263761-01-9P 263761-02-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of 7-substituted tetracycline derivs.)

RN 263760-96-9 CAPLUS
 CN 2-Naphthacene-carboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-phenyl-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

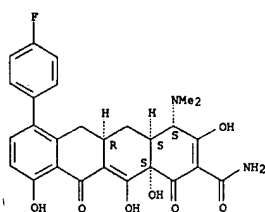
Absolute stereochemistry.



RN 263760-98-1 CAPLUS
 CN 2-Naphthacene-carboxamide, 4-(dimethylamino)-7-(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

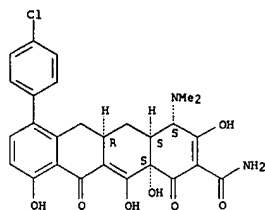
Absolute stereochemistry.

L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 263760-99-2 CAPLUS
 CN 2-Naphthacene-1,11-dione-3,10,12-tetrahydroxy-7-(4-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

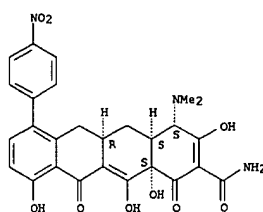
Absolute stereochemistry.



RN 263761-01-9 CAPLUS
 CN 2-Naphthacene-1,11-dione-3,10,12-tetrahydroxy-7-(4-nitrophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

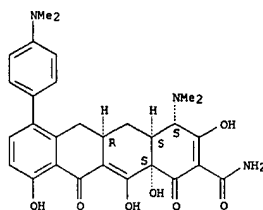
Absolute stereochemistry.

L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 263761-02-0 CAPLUS
 CN 2-Naphthacene-1,11-dione-3,10,12-tetrahydroxy-7-(4-(dimethylamino)phenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 1 OF 1 SCISEARCH COPYRIGHT 2002 ISI (R)
 AN 2000:239123 SCISEARCH
 GA The Genuine Article (R) Number: 295RT
 TI Synthesis of 7-substituted tetracycline derivatives
 AU Kosa D J (Reprint)
 CS MT IDA COLL, DEPT SCI & ALLIED HLTH, 777 DEDHAM ST, NEWTON, MA 02459
 (Reprint)
 CYA USA
 SO ORGANIC LETTERS, (23 MAR 2000) Vol. 2, No. 6, pp.
 815-817.
 Publisher: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036.
 ISSN: 1523-7060.
 DT Article; Journal
 FS PHYS
 LA English
 REC Reference Count: 15
 AB The synthesis of 7-substituted tetracycline derivatives has been
 accomplished in high yield from 7-halotetracyclines by modified Suzuki and
 Stille coupling protocols. These novel derivatives may serve as a new
 class of tetracycline antibiotics effective against multi-antibiotic-
 resistant bacteria.
 CC CHEMISTRY, ORGANIC
 RE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)
BEERBOOM J J	1960	182	1003	J AM CHEM SOC
BOOTHE J H	1960	182	1253	J AM CHEM SOC
BROSHARD R W	1949	109	199	SCIENCE
BROWN A G	1992	1	123	J CHEM SOC PERK T 1
BUCHWALD S L	1998	120	1972	J AM CHEM SOC
FINLAY A C	1950	111	185	SCIENCE
HLAVKA J J	1962	184	1426	J AM CHEM SOC
MCCORMICK J R D	1953	1	181	ANTIBIOT ANNU
MITSCHE L A	1978	19	1	CHEM TETRACYCLINE AN
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PETIST J	1962	15	1538	J MED CHEM
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STILLE J K	1986	125	1508	ANGEW CHEM INT EDIT
VANHONWELING C D	1969	1	121	PAPERS

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FILE 'REGISTRY' ENTERED AT 07:12:57 ON 01 AUG 2002

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L7 0 S L3

FILE 'BEILSTEIN' ENTERED AT 07:17:29 ON 01 AUG 2002

L8 5 S L1 FULL

FILE 'SCISEARCH' ENTERED AT 07:18:31 ON 01 AUG 2002

L9 1 S KOZA?/AU AND 2000/PY AND 2/SO AND 815/SO